# Material Dynamics at Extreme Conditions

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Fig. 1. Incipient spall failure in a copper bicrystal (shocked left-to-right) by homogeneous void nucleation along the (vertical) plane of maximum tensile stress. Only undercoodinated surface atoms are shown, so that one sees the free surfaces of the impactor and target and the voids that have begun to nucleate, grow, and coalesce. The (horizontal) grain boundaries, one in the center of the sample and the other at the top/bottom periodic boundary, remain intact and are not visible.
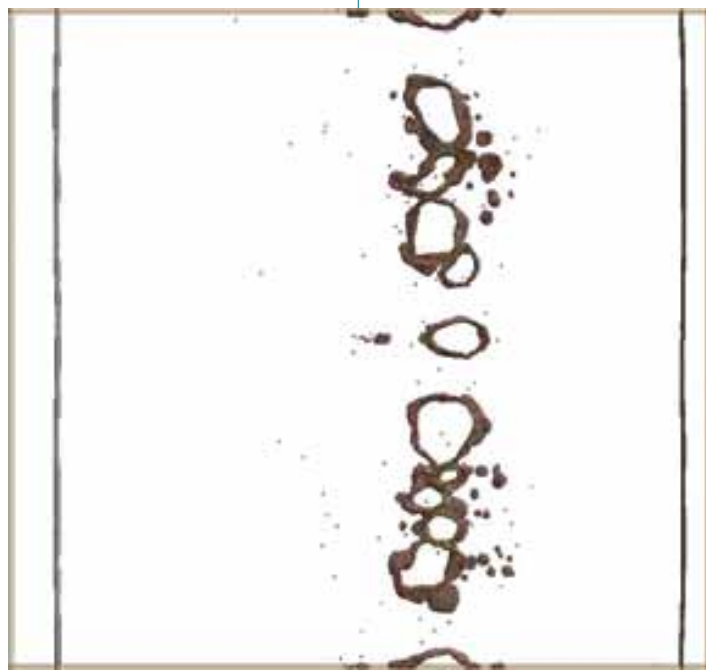
Dynamic loading, such as high-speed sliding friction or shock impact, can dramatically affect the microstructure and properties of materials on ultrafast timescales that are difficult–if not impossible–to probe experimentally. Because sound waves travel at a few km/s, or equivalently a few nm/ps, through a typical metal, they traverse the sub-nm interatomic lattice spacing in much less than a picosecond (ps). While experimentally challenging, processes occurring at such nm length and ps time scales are ideal for study by nonequilibrium molecular dynamics (MD) simulations. Over the past decade, large-scale MD simulations have provided significant insight into the microscopic pathways and kinetics of shock-induced plasticity and phase transformations in single-crystal metals. Sample sizes of a few million atoms are typically sufficient; representing a cube of material with edge lengths 10-100 nm, this can capture the emergent length scale (average spacing between dislocations or product phase nuclei). Such simulations first suggested that the polymorphic (bcc-hcp) transformation in shocked iron can take place on ps timescales [1]. The predicted orientation relationship, timescale, and product grain size were all subsequently confirmed by ultrafast in situ X-ray diffraction measurements on laser-shocked iron thin foils [2].

The SPaSM (Scalable Parallel Short-range Molecular Dynamics) code was originally developed in the early 1990s for the newly emerging era of massively parallel supercomputers such as the Thinking Machines CM-5, and achieved IEEE Gordon Bell Prize-winning performance by minimizing memory usage and floating-point operations. However, for the modern generation of heterogeneous, multicore architectures such as Roadrunner, it is data movement rather than storage or arithmetic operations that is increasingly the bottleneck. Thus, we have redesigned the entire communication infrastructure and data structures of SPaSM to allow for better asynchrony between the processors, in particular to accommodate the IBM Cell BroadBand Engine (Cell BE) processor and the unique multilayer hierarchy of Roadrunner's architecture. This effort has paid off, resulting in double-precision benchmark performance of 369 TFlop/s on the full machine [3], and a ~5x speedup for the embedded atom method (EAM) potentials typically used to model simple metals such as copper, silver, and iron.

Using the SPaSM code on Roadrunner, we are investigating the ejection of material that can occur from shocked surfaces [4]. The goal of this work is to develop models that can predict the amount of mass ejected from a shocked interface with a given surface finish and loading history (peak shock pressure, either from a supported square-wave or explosive-driven Taylor wave). We would also like to understand how that mass is distributed, namely its particle size and velocity distributions, as well as evolutions and correlations, if any, between the two. Experimentally, the total mass can be inferred by measuring the resulting momentum transfer onto an Asay foil or piezoelectric probe at some standoff distance, while particle sizes larger than a micron can be imaged using holography or X-ray radiography. However, there is no direct experimental information on the distribution of particle sizes smaller than a micron, nor on the correlation between size and velocity distributions.

On such microscopic scales, MD simulations can complement experiments by providing unique insight into the material dynamics at submicron length and subnanosecond timescales, including key fragmentation and atomization mechanisms, but until now this problem had remained computationally intractable. The

formation and transport of ejecta involves a complex range of physical processes, including Richtmyer-Meshkov instability (RMI) development in solid materials with dynamic material strength properties, classical and turbulent fragmentation and atomization, and particulate transport in a turbulent gas. We have carried out a systematic study of RMI development from a single sinusoidal surface perturbation in copper to test various RMI theories including material strength effects, which suppress the instability growth. We are using these simulations to study the evolution of the density and velocity distributions of the ejected mass, the modes of particle breakup, and ultimately to develop source theories of ejecta formation based on RMI growth, including material strength effects and transport models that describe the temporally evolving particle size and velocity distributions. Earlier MD simulations were able to demonstrate the initial jet formation but could not reach timescales long enough to observe the subsequent necking instabilities leading to jet breakup and droplet formation that have now been revealed (Fig. 1). These fragmentation and atomization processes are also difficult to study experimentally, although various theories have been proposed; atomistic-level simulations such as those presented here are contributing to the development of physics-based models at LANL.

Ejecta is only one form of shock-induced material failure, occurring when a shock wave reflects from a free surface to become an expanding rarefaction (or release) fan. When two such rarefaction fans (one from the impactor free surface, the other from the target) intersect in the interior of the material, they put the material into tension and can lead to spall failure [5]. Ductile spall failure results from the nucleation, growth, and coalescence of voids; models have been developed that account for each of these aspects, but without direct experimental information; due again to the ultrafast time and ultrasmall length scales. Using Roadrunner, we have been able to study this process in copper bicrystals, revealing the competition between heterogeneous void nucleation at defects such as grain boundaries (GB) and homogeneous nucleation within the bulk single crystal. Large system sizes are required to clearly separate the two processes, and long timescales to explore a wide range of

strain rates. Figure 2 shows a Cu bicrystal loaded parallel to the horizontal GBs (one in the center and the other at the top/bottom periodic boundary), with 400 m/s impact velocity. The sample is 230 nm tall (i.e., each grain is 115 nm), 20-nm thick (into the plane, i.e., images are looking through the entire 20-nm thickness), and 205-nm long (54 million atoms in all). Following shock compression and release, dislocations and voids are produced that leave the sample in an incipient spall state; that is, with a number of voids that remain intact after growing and coalescing, but that have not caused complete fragmentation. In this example, the short sample length leads to a very high strain rate, with voids primarily nucleated homogeneously (within the grains) along the vertical plane of maximum tensile stress. On the other hand, a longer sample length (1 µm, 270 million atoms) leads to a lower strain rate and sufficient time for void nucleation to be localized at the GBs, changing the failure mode from a vertical spall plane to a horizontal grain decohesion. These results indicate the interplay between grain size and the timescale for nucleation kinetics, with a competition between heterogeneous and homogeneous nucleation.

Fig. 2. Incipient spall failure in a copper bicrystal by heterogeneous void nucleation along the (horizontal) grain boundaries.

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